IN THE CLAIMS:

This listing of claims replaces all prior versions and listings of claims in the application:

Listing of Claims

Claims 1-8. (Canceled)

9. (Currently Amended) A computer-assisted method for determining a three-dimensional structure of a target protein using a computer comprising a processor configured to receive and output data in accordance with executable code thereon, the executable code causing the computer to ~~method comprising~~:

~~(a) generating input data for the computer comprising:~~

(i) ~~inputting~~ obtain, as a string, an identity constraint and a secondary structure constraint and/or tertiary constraints for some or all of the amino acid residues ~~residue~~ comprising the target protein; ~~and~~

(ii) ~~by way of executable code, directing the processor to produce~~ align the amino acid residues of the target protein with amino acid residues of a template protein;

(iii) define a virtual interaction center for each amino acid side chain of the target protein by identifying a center of mass of a side chain of an amino acid and identifying the center of mass as the virtual interaction center;

(iv) produce from the string ~~a three dimensional reduced protein model comprised of~~ representations of side chains of the amino acid residues comprising the target protein wherein said representations of side chains of amino acid residues are ~~converted to interaction centers and each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and~~ represented by each interaction center, wherein each interaction center is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to

produce an interaction center chain~~, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers,~~;

(vi) apply~~, and then~~ secondary constraints and/or tertiary constraints ~~are applied~~ to a subset of, or all of, the interaction centers of the interaction center chain to generate a knowledge based origin ~~comprising~~ defined by a virtual force field of short-range interactions;

(vii) sequentially project each interaction center onto an underlying virtual cubic lattice to produce a projected chain of interaction centers beginning with a first aligned position of the target and template amino acid sequence and each subsequent interaction center selected so as to minimize the distance of the projected chain of interaction centers from an equivalent template chain and limited by the knowledge based origin, and wherein a gap in the alignment is defined as a checkpoint, wherein the checkpoint is the distance from the last aligned residue to the next aligned residue divided by the number of non-aligned residues such that the number of checkpoints is equal to the number of target sequence residues that have to be mounted to span the gap;

(viii) produce~~, thereby producing~~ a ~~data set representing~~ a three-dimensional model structure of the target protein defined by the projected chain of interaction centers; and

(b) output~~ting~~ the three dimensional ~~reduced protein~~ model structure to an output device or a storage device.

10. (Original) A method according to claim 9 wherein the secondary structure constraint for each amino acid residue is selected from the group of "H" for helix, "E" for extended, and "(i)" for other structural constraints.

11. (Original) A method according to claim 9 wherein the secondary structural constraint for a subset of amino acid residues comprising the target protein is generated by a threading alignment of an amino acid sequence of the target protein.

Claims 12-13. (Canceled)